Amendments to the Claims

Pursuant to 37 C.F.R. § 1.121(c), this listing of claims will replace all prior versions, and listing of claims in the application:

1. (currently amended) A computer-implemented method for use in deriving a chemical structure diagram, comprising:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;

~~positioning~~ laying out symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry; and

outputting a representation of chemical structure.

2. (withdrawn) A method for use in deriving a chemical structure diagram, comprising:

determining, from a first chemical structure diagram, a force term for increasing diagrammatic symmetry within the first chemical structure diagram, the force term being based on the difference between an optimal angle and a current angle; and

applying the force term in a derivation of a second chemical structure diagram from the first chemical structure diagram, the second chemical structure diagram having more diagrammatic symmetry than the first chemical structure diagram.

3. (withdrawn) A method for use in deriving a chemical structure diagram, comprising:

determining, from a first chemical structure diagram, a parameter for use in producing the shape of an addition to the first chemical structure diagram;

producing the shape of the addition based on the parameter, the addition including a bridge addition to the first chemical structure diagram; and

producing a second chemical structure diagram by adding the addition to the first chemical structure diagram.

4. (withdrawn) A method for use in deriving a chemical structure diagram, comprising:

keeping track of unused display area;

determining a first rectangle that defines a first portion of an available layout area within the unused display area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram;

determining a second rectangle that defines a second portion of an available layout area, the second portion being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

positioning the first and second chemical structure diagrams within the first and second portions, respectively.

5. (currently amended) A system for use in deriving a chemical structure diagram, comprising:

an identifier identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure, wherein the instance of chemical structural symmetry includes symmetrically equivalent atoms and bonds; and

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds; and

a positioner ~~positioning~~ laying out symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry; and

an output device outputting a representation of chemical structure.

6. (withdrawn) A system for use in deriving a chemical structure diagram, comprising:

a determiner determining, from a first chemical structure diagram, a force term for increasing diagrammatic symmetry within the first chemical structure diagram, the force term being based on the difference between an optimal angle and a current angle; and

an applicator applying the force term in a derivation of a second chemical structure diagram from the first chemical structure diagram, the second chemical structure diagram having more diagrammatic symmetry than the first chemical structure diagram.

7. (withdrawn) A system for use in deriving a chemical structure diagram, comprising:

a determiner determining, from a first chemical structure diagram, a parameter for use in producing the shape of an addition to the first chemical structure diagram; and

a producer producing the shape of the addition based on the parameter, the addition including a bridge addition to the first chemical structure diagram, and producing a second chemical structure diagram by adding the addition to the first chemical structure diagram.

8. (withdrawn) A system for use in deriving a chemical structure diagram, comprising:

a tracker keeping track of available display area;

a determiner determining a first rectangle that defines a first portion of an available layout area within the unused display area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram, the determiner determining a second rectangle that defines a second portion of an available layout area, the second portion being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

a positioner positioning the first and second chemical structure diagrams within the first and second portions, respectively.

9. (currently amended) Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

identify, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure, wherein the instance of chemical structural symmetry includes symmetrically equivalent atoms and bonds; and

~~wherein the instance of symmetry includes symmetrically equivalent atoms and bonds; and~~

~~position~~ lay out symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry; and

output a representation of chemical structure.

10. (withdrawn) Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

determine, from a first chemical structure diagram, a force term for increasing diagrammatic symmetry within the first chemical structure diagram, the force term being based on the difference between an optimal angle and a current angle; and

apply the force term in a derivation of a second chemical structure diagram from the first chemical structure diagram, the second chemical structure diagram having more diagrammatic symmetry than the first chemical structure diagram.

11. (withdrawn) Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

determine, from a first chemical structure diagram, a parameter for use in producing the shape of an addition to the first chemical structure diagram;

produce the shape of the addition based on the parameter, the addition including a bridge addition to the first chemical structure diagram; and

produce a second chemical structure diagram by adding the addition to the first chemical structure diagram.

12. (withdrawn) Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

keep track of unused display area;

determine a first rectangle that defines a first portion of an available layout area within the unused display area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram;

determine a second rectangle that defines a second portion of an available layout area, the second portion being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

position the first and second chemical structure diagrams within the first and second portions, respectively.

13. (previously presented) The method of claim 1, wherein the instance of chemical structural symmetry is based on rotational symmetry.

14. (previously presented) The method of claim 1, wherein the instance of chemical structural symmetry is based on reflective symmetry.

15. (previously presented) The method of claim 1, wherein the instance of chemical structural symmetry is based on inversive symmetry.

16. (previously presented) The method of claim 1, further comprising:

basing the identification on stereochemistry.

17. (previously presented) The method of claim 1, further comprising:

basing the identification on rotational symmetry, reflective symmetry, and stereochemistry.

18. (previously presented) The method of claim 1, further comprising:

basing the identification on double bond stereochemistry.

19. (previously presented) The method of claim 1, further comprising:

determining a pivot point for the list.

20. (previously presented) The method of claim 1, further comprising:

determining a graph-theoretic center for the list.

21. (previously presented) The method of claim 1, further comprising:

determining a symmetric order for the instance of chemical structural symmetry.

22. (previously presented) The method of claim 1, further comprising:

determining whether an atom belongs to the identified instance of chemical structural symmetry.

23. (previously presented) The method of claim 1, further comprising:

determining whether a bond belongs to the identified instance of chemical structural symmetry.

24. (previously presented) The method of claim 1, further comprising:

in the event the identified instance of chemical structural symmetry is reflective, selecting a position on an opposite side of a mirror line.

25. (previously presented) The method of claim 1, further comprising:

in the event the identified instance of chemical structural symmetry is rotative, selecting a position based on a pivot point.

26. (previously presented) The method of claim 1, further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is horizontal.

27. (previously presented) The method of claim 1, further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is vertical.

28. (new) A computer-implemented method for use in deriving a chemical structure diagram, comprising:

identifying an instance of chemical structural symmetry in the chemical structure;

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;

laying out symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry; and

outputting a representation of chemical structure.

29. (new) The method of claim 28, wherein the instance of chemical structural symmetry is based on rotational symmetry.

30. (new) The method of claim 28, wherein the instance of chemical structural symmetry is based on reflective symmetry.

31. (new) The method of claim 28, wherein the instance of chemical structural symmetry is based on inversive symmetry.

32. (new) The method of claim 28, further comprising:

basing the identification on stereochemistry.

33. (new) The method of claim 28, further comprising:

basing the identification on rotational symmetry, reflective symmetry, and stereochemistry.

34. (new) The method of claim 28, further comprising:

basing the identification on double bond stereochemistry.

35. (new) A system for use in deriving a chemical structure diagram, comprising:

an identifier identifying an instance of chemical structural symmetry in the chemical structure, wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;

a positioner laying out symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry; and

an output device outputting a representation of chemical structure.